

1/30/06

US 2000-233087P P 20000915  
US 2000-234816P P 20000922  
US 2001-957654 A3 20010917

FAN 2002:332188

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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search*

1/30/06

US 2000-232891P P 20000915  
 US 2000-234510P P 20000922  
 US 2001-957682 A3 20010917

PATENT FAMILY INFORMATION:

FAN 2002:220575

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10799386

1/30/06

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OS MARPAT 136:263160  
IT 405172-14-7P 405172-81-8P 405172-82-9P  
405172-83-0P 405172-84-1P 405173-01-5P  
405173-02-6P 405173-43-5P 405173-45-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

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1/30/06

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(preparation of azolylmethylaninotetrahydroquinolines and related compds. as  
chemokine receptor binding agents)

RN 405172-14-7 CAPLUS

CN 1,4-Benzenedimethanamine, N,N'-bis(1H-benzimidazol-2-ylmethyl)-N,N'-  
bis(5,6,7,8-tetrahydro-8-quinolinyl)-, tetrahydrobromide (9CI) (CA INDEX  
NAME)

1/30/06

US 2005026942 A1 20050203

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US 2001-957682 A3 20010917  
US 2004-914663 20040809  
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PATENT FAMILY INFORMATION:

FAN 2002:220575

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1/30/06

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1/30/06

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10221446

1/30/06

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1/30/06

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NEWS 4 DEC 14 2006 MeSH terms loaded in MEDLINE/LMEDLINE  
NEWS 5 DEC 14 2006 MeSH terms loaded for MEDLINE file segment of TOXCENTER  
NEWS 6 DEC 14 CA/CAPLUS to be enhanced with updated IPC codes  
NEWS 7 DEC 21 IPC search and display fields enhanced in CA/CAPLUS with the  
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NEWS 12 JAN 17 IPC 8 in the WPI family of databases including WPIFV  
NEWS 13 JAN 30 Saved answer limit increased

NEWS EXPRESS JANUARY 03 CURRENT VERSION FOR WINDOWS IS V8.01,  
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.  
V8.0 USERS CAN OBTAIN THE UPGRADE TO V8.01 AT  
<http://download.cas.org/express/v8.0-Discover/>

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NEWS INTER General Internet Information  
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NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

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FULL ESTIMATED COST	0.21	0.21

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\*  
\*\*\*\*\*

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=>

Uploading C:\Program Files\Stnexp\Queries\10799386-2.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful

FULL SEARCH INITIATED 12:10:22 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 13621 TO ITERATE

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100.0% PROCESSED 13621 ITERATIONS  
SEARCH TIME: 00.00.01

86 ANSWERS

L2 86 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

167.38

167.59

FILE 'CAPLUS' ENTERED AT 12:10:26 ON 31 JAN 2006

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FILE COVERS 1907 - 31 Jan 2006 VOL 144 ISS 6

FILE LAST UPDATED: 30 Jan 2006 (20060130/ED)

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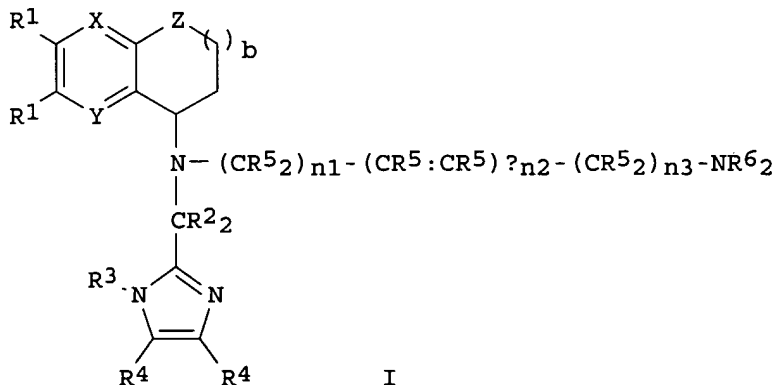
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L3 3 L2

=> d abs bib fhitr 1-3

L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

GI



10799386

1/30/06

AB The invention relates to heterocyclic compds. (shown as I; e.g. (1H-benzimidazol-2-ylmethyl)(piperidin-3-ylmethyl)(5,6,7,8-tetrahydroquinolin-8-yl)amine trihydrobromide) consisting of a core N atom surrounded by three pendant groups, wherein two of the three pendant groups are preferably benzimidazolylmethyl and tetrahydroquinolyl, and the 3rd pendant group contains N and optionally contains addnl. rings. The compds. bind to chemokine receptors, including CXCR4 and CCR5, and demonstrate protective effects against infection of target cells by a human immunodeficiency virus (HIV). Many I exhibit IC50 values of 5-5.5 nM for inhibition of HIV-1 (NL4.3) replication in peripheral blood mononuclear cells and 5 nM-5 µM for inhibition of SDF-1α induced Ca flux in CCRF-CEM cells, a T-lymphoblastoid cell line that expresses CXCR4. It is also stated that the compds. I behave in a manner similar to 1,1'-[1,4-phenylene-bis(methylene)]-bis-1,4,8,11-tetraazacyclotetradecane (AMD3100) which showed to elevate progenitor cell levels (data given). Although the methods of preparation are not claimed, >170 example preps. are included. For I: X and Y = N or CR1; Z is S, O, NR1 or CR12; each R1-R6 = H or a noninterfering substituent; n1 is 0-4; n2 is 0-1, wherein the a signifies C.tplbond.C may be substituted for CR5:CR5; n3 is 0-4; wherein n1 + n2 + n3 = ≥ 2; b is 0-2; wherein the following combinations of R groups may be coupled to generate a ring, which ring may be (un)saturated: R2 + R2, one R2 + R3, R3 + one R4, R4 + R4, one R5 + another R5, one R5 + one R6, and R6 + R6; wherein the ring may not be aromatic when the participants in ring formation are two R5; and wherein when n2 is 1, neither n1 nor n3 can be 0.

AN 2004:80349 CAPLUS

DN 140:146136

TI Preparation of chemokine receptor binding (benzimidazol-2-ylmethyl)(5,6,7,8-tetrahydroquinolin-8-yl)amines and related heterocyclic compounds with enhanced efficacy against AIDS and other disorders

IN Bridger, Gary; Kaller, Al; Harwig, Curtis; Skerlj, Renato; Bogucki, David; Wilson, Trevor R.; Crawford, Jason; McEachern, Ernest J.; Atsma, Bem; Nan, Siqiao; Zhou, Yuanxi; Schols, Dominique; Smith, Christopher D.; Di Fluri, Maria R.

PA USA

SO U.S. Pat. Appl. Publ., 154 pp., Cont.-in-part of U.S. Ser. No. 446,170. CODEN: USXXCO

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004019058	A1	20040129	US 2003-457034	20030606
	US 2003220341	A1	20031127	US 2002-329329	20021223
	WO 2004106493	A2	20041209	WO 2004-US15977	20040521
	WO 2004106493	A3	20050825		
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PRAI US 2001-342716P P 20011221

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US 2002-350822P	P	20020117
US 2002-329329	A2	20021223
US 2003-446170	A2	20030523
US 2003-457034	A	20030606

OS MARPAT 140:146136

IT 558441-51-3P

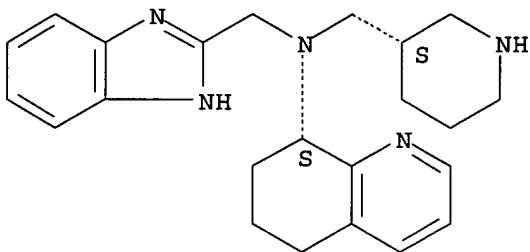
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of chemokine receptor binding benzimidazolylmethyl tetrahydroquinolinyl amines and related heterocyclic compds. with enhanced efficacy against AIDS and other disorders)

RN 558441-51-3 CAPLUS

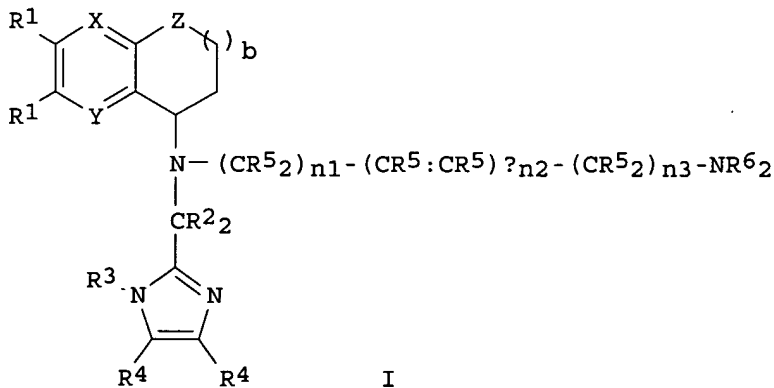
CN 8-Quinolinamine, N-(1H-benzimidazol-2-ylmethyl)-5,6,7,8-tetrahydro-N-[(3R)-3-piperidinylmethyl]-, trihydrobromide, (8R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● 3 HBr

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN  
GI



I

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AB The invention relates to heterocyclic compds. (shown as I; e.g. (1H-benzimidazol-2-ylmethyl)(piperidin-3-ylmethyl)(5,6,7,8-tetrahydroquinolin-8-yl)amine trihydrobromide) consisting of a core N atom surrounded by three pendant groups, wherein two of the three pendant groups are preferably benzimidazolylmethyl and tetrahydroquinolyl, and the 3rd pendant group contains N and optionally contains addnl. rings. The compds. bind to chemokine receptors, including CXCR4 and CCR5, and demonstrate protective effects against infection of target cells by a human immunodeficiency virus (HIV). Many I exhibit IC50 values of 5-5.5 nM for inhibition of HIV-1 (NL4.3) replication in peripheral blood mononuclear cells and 5 nM-5 µM for inhibition of SDF-1α induced Ca flux in CCRF-CEM cells, a T-lymphoblastoid cell line that expresses CXCR4. Although the methods of preparation are not claimed, >170 example preps. are included. For I: X and Y = N or CR1; Z is S, O, NR1 or CR12; each R1-R6 = H or a noninterfering substituent; n1 is 0-4; n2 is 0-1, wherein the a signifies C.tplbond.C may be substituted for CR5:CR5; n3 is 0-4; wherein n1 + n2 + n3 = ≥ 2; b is 0-2; wherein the following combinations of R groups may be coupled to generate a ring, which ring may be (un)saturated: R2 + R2, one R2 + R3, R3 + one R4, R4 + R4, one R5 + another R5, one R5 + one R6, and R6 + R6; wherein the ring may not be aromatic when the participants in ring formation are two R5; and wherein when n2 is 1, neither n1 nor n3 can be 0.

AN 2003:532661 CAPLUS

DN 139:101128

TI Preparation of chemokine receptor binding (benzimidazol-2-ylmethyl)(5,6,7,8-tetrahydroquinolin-8-yl)amines and related heterocyclic compounds with enhanced efficacy against AIDS and other disorders

IN Bridger, Gary J.; Skerlj, Renato T.; Kaller, Al; Harwig, Curtis; Bogucki, David; Wilson, Trevor; Crawford, Jason; McEachern, Ernest J.; Atsma, Bem; Nan, Sigiao; Zhou, Yuanxi; Schols, Dominique; Smith, Christopher Dennis; Di Fluri, Rosaria Maria

PA Anormed Inc., Can.; et al.

SO PCT Int. Appl., 360 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

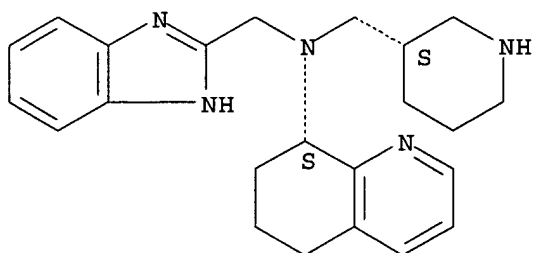
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	AU 2002357379	A1	20030715	AU 2002-357379	20021223
	BR 2002015050	A	20041013	BR 2002-15050	20021223
	EP 1465889	A1	20041013	EP 2002-805977	20021223
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	JP 2005518397	T2	20050623	JP 2003-556406	20021223
	NO 2004002578	A	20040907	NO 2004-2578	20040618
PRAI	US 2001-342716P	P	20011221		

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US 2002-350822P P 20020117  
WO 2002-US41407 W 20021223  
OS MARPAT 139:101128  
IT 558441-51-3P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)  
(drug candidate; preparation of chemokine receptor binding  
benzimidazolylmethyl tetrahydroquinoliny l amines and related  
heterocyclic compds. with enhanced efficacy against AIDS and other  
disorders)  
RN 558441-51-3 CAPLUS  
CN 8-Quinolinamine, N-(1H-benzimidazol-2-ylmethyl)-5,6,7,8-tetrahydro-N-[(3R)-  
3-piperidinylmethyl]-, trihydrobromide, (8R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



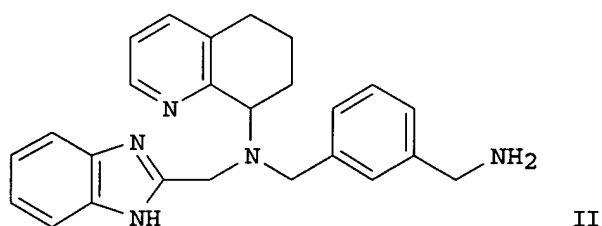
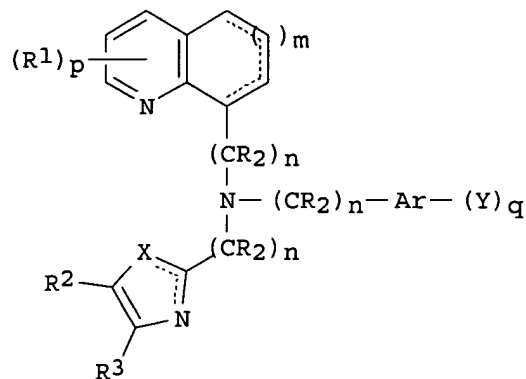
● 3 HBr

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN  
GI



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AB Title compds. I [wherein ring A optionally comprises a heteroatom selected from N, O, or S; R1-R3 = non-interfering substituents; R4 and R5 = independently H or (un)substituted alkyl, alkenyl, alkynyl, or acyl; or 2 R5 may form a cyclic amine, optionally containing 1 or more N, O, and/or S; R = independently H or alkyl; X = O or S or (un)substituted C or N; Y = independently halo, OH, SH, SO, SO2, non-N containing organic moiety, (CH2)xCN, (CR2)xNR52, (CR2)xNR(CR2)xNRR4, (CR2)xNR(CR2)xNR(CR2)xNR52, (CR2)xCO(CR2)xNR52, (CR2)xCO(CR2)xNR(CR2)xNRR4, (CR2)xCO(CR2)xNR(CR2)xNR(CR2)xNR52, (CR2)xNRCO(CR2)xNRR4, (CR2)xNRCO(CR2)xNR(CR2)xNR52, (CR2)xNRCO(CR2)xNR(CR2)xNR(CR2)xNR(CR2)xNR52, CH:NZ, (CR2)xZ, NR(CR2)xZ, (CR2)xNROH, (CR2)xCONROH, or (CR2)xCR:NOH; or 2 Y groups may be connected to form a fused ring with Ar; Z = (un)substituted (hetero)aryl; Ar = (hetero)aryl; m = 0-2; n = 0-2; p = 0-4; q = 0-3; x = 0-4; with provisos; and pharmaceutically acceptable salts and pro-drugs thereof] were prepared as modulators of chemokine receptor activities. For example, reductive addition of 3-cyanobenzaldehyde to 8-amino-5,6,7,8-tetrahydroquinoline using sodium triacetoxyborohydride in CH2Cl2 afforded N-(5,6,7,8-tetrahydro-8-quinolinyl)-3-cyanobenzylamine (81%). Alkylation with N-(tert-butoxycarbonyl)-2-chloromethylbenzimidazole using N,N-diisopropylethylamine and KI in MeCN (88%), followed by hydrogenation in the presence of Raney nickel (79%), gave the tertiary amine II (AMD9679). Compds. of the invention tested for inhibition of HIV-1 NL4.3 or IIIB replication in MT-4 cells exhibited EC50 values of 0.002  $\mu$ M/mL to 20.0  $\mu$ M/mL. Thus, I are useful for the treatment of human immunodeficiency virus (HIV) and/or feline immunodeficiency virus (FIV).

AN 2002:332188 CAPLUS

DN 136:355235

TI Preparation of tertiary N-(5,6,7,8-tetrahydro-8-quinolinyl)-N-(1H-benzimidazol-2-ylmethyl)amines and analogs as chemokine receptor modulators for treatment of HIV or FIV

IN Bridger, Gary; Skerlj, Renato; Kaller, Al; Harwig, Curtis; Bogucki, David;

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1/30/06

Wilson, Trevor R.; Crawford, Jason; Mceachern, Ernest J.; Atsman, Berm;  
Nan, Sigiao; Zhou, Yuanxi; Schols, Dominique; Smith, Christopher Dennis;  
Di Fluri, Rosaria Maria

PA Anormed Inc., Can.

SO PCT Int. Appl., 187 pp.

CODEN: PIXXD2

DT Patent

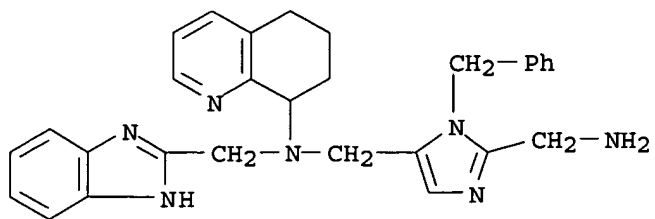
LA English

FAN.CNT 3

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	EP 1317451	A1	20030611	EP 2001-975290	20010917
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	AU 2001094628	A5	20020506	AU 2001-94628	20010919
	JP 2004512336	T2	20040422	JP 2002-537736	20010919
	US 2003028022	A1	20030206	US 2002-31812	20020328
	US 6734191	B2	20040511		
	NO 2003001161	A	20030313	NO 2003-1161	20030313
	US 2004171638	A1	20040902	US 2004-799386	20040311
	US 2004220207	A1	20041104	US 2004-858910	20040601
	US 2005026942	A1	20050203	US 2004-914663	20040809
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	US 2000-234816P	P	20000922		
	US 2000-232891P	P	20000915		
	US 2000-233087P	P	20000915		
	US 2001-957654	A3	20010917		
	US 2001-957682	A3	20010917		
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	US 2002-31812	A1	20020328		
OS	MARPAT 136:355235				
IT	422282-07-3P, AMD 9986				
	RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)				
	(chemokine receptor modulator; preparation of N-(tetrahydroquinolinyl)-N-(benzimidazolylmethyl)amines and analogs as chemokine receptor modulators for treatment of HIV or FIV)				
RN	422282-07-3 CAPLUS				
CN	1H-Imidazole-2,5-dimethanamine, N5-(1H-benzimidazol-2-ylmethyl)-1-(phenylmethyl)-N5-(5,6,7,8-tetrahydro-8-quinolinyl)-, tetrahydrobromide (9CI) (CA INDEX NAME)				

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1/30/06



●4 HBr

RE.CNT 6      THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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